

Dimethyl glutarate

1119-40-0 | DTXSID3025122

Model Performance

| | |
|-------|------|
| Model | Data |
|-------|------|

Weighted KNN model

| 5-fold CV (75%) | | Training (75%) | | Test (25%) | |
|-----------------|------|----------------|------|------------|------|
| Q2 | RMSE | R2 | RMSE | R2 | RMSE |
| 0.85 | 1.14 | 0.85 | 1.12 | 0.83 | 1.23 |

Model Results

Predicted value: 3.76×10^{-12} cm³/molecule*sec

Global applicability domain: Inside

Local applicability domain index: 6.36×10^{-1}

Confidence level: 7.39×10^{-1}

Nearest Neighbors from the Training Set

Image not found

Dimethyl glutarate

Measured: 3.30×10^{-12}

Predicted: 3.76×10^{-12}

Image not found

Dimethyl adipate

Measured: 8.40×10^{-12}

Predicted: 6.84×10^{-12}

Image not found

Dimethyl succinate

Measured: 1.40×10^{-12}

Predicted: 1.93×10^{-12}

Image not found

Ethyl 3-ethoxypropionate

Measured: 2.29×10^{-11}

Predicted: 1.63×10^{-11}

Image not found

2-Ethoxyethyl acetate

Measured: 1.30×10^{-11}

Predicted: 1.03×10^{-11}